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Boundary Conditions as Dirac Constraints

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Abstract

In this article we show that boundary conditions can be treated as Lagrangian and Hamiltonian primary constraints. Using the Dirac method, we find that boundary conditions are equivalent to an infinite chain of second class constraints which is a new feature in the context of constrained systems. We discuss the Dirac brackets and the reduced phase space structure for different boundary conditions. We also show that in a quantized field theory subjected to the mixed boundary conditions, the field components are noncommutative.

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1 Introduction

It is well-known that to formulate a general classical field theory defined in a box, besides the equations of motion we should know the behaviour of the fields on the boundaries, boundary conditions. Boundary conditions are usually relations between the fields and their various derivatives, containing the time derivative, on the boundaries, expected to be held at all the times. In Hamiltonian language the boundary conditions are in general functions of the fields and their conjugate momenta; hence the field theories subjected to the boundary conditions might be understood by the prescription for handling the constrained systems proposed by Dirac [1].

In the usual field theory arguments, since boundary conditions are generally a linear combination of fields and their momenta, one can easily impose them on the solutions of the equations of motion, and find the final result. But, imposing the boundary conditions in some special cases may lead to inconsistencies with the canonical commutation relations [2, 3, 5, 4, 6, 7].

In this article, considering the boundary conditions as constraints, we apply the Dirac's procedure to this constrained system. Although this idea have been used in [5, 6], the problem has new and special features in the context of constrained systems on which, we mostly concentrate.

In the second section, we review the Lagrangian and Hamiltonian constrained systems. In section 3, to visualize the seat of boundary conditions we take a toy model and by discretizing the model show that boundary conditions are in fact the equations of motion for the points at the boundaries. In section 4, going to Hamiltonian picture we study the constraint structure resulting from the boundary conditions, and apply it explicitly to some field theories. The new feature of this constraint structure is, the infinite chain of second class constraints. In section 5, building the Dirac bracket structure we briefly study the quantized theory. We also compare our results with the mode expansions and discuss that, using the proper mode expansions is the same as going to *reduced phase space*. In section 6, we apply the machinery developed in previous sections to the case of mixed boundary conditions, i.e. , we find the constraints chain, the Dirac bracket and the reduced phase space. The new and interesting result of this case is that, the Dirac bracket of two field components is obtained to be non-zero and hence, in the quantum theory these field components are noncommuting. The last section is devoted to the concluding remarks.

2 Review of Dirac Procedure

Given the Lagrangian $L(q, \dot{q})$ (or $L(\phi, \partial\phi)$ in a field theory), the Lagrangian equations of motion are:

$$\mathbf{L}_i = W_{ij}\ddot{q}_j + \alpha_i = 0, \tag{2.1}$$

where $\mathbf{L}_i$ are Eulerian derivatives, $W_{ij}(q, \dot{q}) = \frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j}$ is called the Hessian matrix, and $\alpha_i = \frac{L}{\partial q^i} - \dot{q}_j(\frac{L}{\partial \dot{q}^i \partial q^j})$. If $|W_{ij}| = 0$, the Lagrangian is *singular* and in this case the number of equations containing accelerations are less than the number of degrees of freedom. Hence a number of Lagrangian constraints, $\gamma^a(q, \dot{q}) = 0$, emerges [2]. Then we should add the time derivatives of constraints,$\dot{\gamma}^a(q, \dot{q})$, to the set of equations of motion to get new relations containing the accelerations. Two cases may happen

1) rank of equations with respect to acceleration is equal to the number of degrees of freedom.
2) new constraints, acceleration free relations, emerging.

In the first case the equations of motion can be solved completely, but solutions should obey the acceleration free equations, the constraints. In the second, the derivatives of new constraints and derivatives of previous constraints should be added to the equations of motion , and the same scenario is repeated.

At the end, there may remain a number of undetermined accelerations; it is shown that they correspond to the gauge degrees of freedom and are related to the first class Hamiltonian constraints. Moreover roughly speaking, there may exist some degrees of freedom which have no dynamics and completely determined via the constraints. These are related to the the second class Hamiltonian constraints [9].

Let us study the Hamiltonian formulation. Singularity of the Hessian matrix, $\frac{p_i}{\partial \dot{q}^j}$, implies the Legendre transformation, $(q, \dot{q}) \to (q, p)$, to have a zero Jacobian and hence, the set of momenta, p_i;

$$p_i = \frac{L}{\partial \dot{q}^i}, \tag{2.2}$$

are not independent functions of q and $\dot{q}$, so a number of Hamiltonian primary constraints turns up

$$\Phi_a^{(0)}(q, p) = 0. \tag{2.3}$$

It can be shown that [1] dynamics of any function in phase space is obtained by

$$\dot{g} \approx \{g, H_T\}_{P.B.}, \tag{2.4}$$

[2]To obtain these constraints we should simply multiply both sides of (2.1) by the null eigenvector λ_i^a of W, so $\gamma^a(q, \dot{q}) = \lambda_i^a \alpha_i$, [8].

where weak equality, $\approx$, is the equality on the constraint surface, and

$$H_T = H + \lambda_a \Phi_a, \tag{2.5}$$

is the total Hamiltonian, λ_a being the Lagrange multipliers.

Like the Lagrangian case the consistency conditions of the primary constraints should be investigated, i.e. the constraints should be valid under the time evolution:

$$\dot{\Phi}_a^{(0)} \approx \{\Phi_a^{(0)}, H_T\}_{P.B.} \approx \{\Phi_a^{(0)}, H\} + \lambda_b\{\Phi_a^{(0)}, \Phi_b^{(0)}\} \approx 0. \tag{2.6}$$

If the above relation dose not hold identically, there are then two possibilities

i) $\{\Phi_a^{(0)}, \Phi_b^{(0)}\}$'s weakly vanish. In this case new Hamiltonian constraints

$$\Phi^{(1)} = \{\Phi_a^{(0)}, H\}, \tag{2.7}$$

turns up.

ii) $\{\Phi_a^{(0)}, \Phi_b^{(0)}\}$ do not vanish, yielding equations on λ_a.

In general, depending on the rank of the matrix $\{\Phi_a^{(0)}, \Phi_b^{(0)}\}$, we may have a mixture of two possibilities. That is some of the Lagrange multipliers are determined and a number of new constraints emerge. Here we do not bother the reader with the details. A complete and detailed discussion can be found in [9].

Now the consistency conditions of $\Phi_a^{(1)}$ should be verified which may result into some new constraints $\Phi_a^{(2)}$. The procedure goes on, and finally we end up with some *constraint chains*. Roughly speaking, each chain terminates if a Lagrange multiplier is determined or, if we get an identically satisfied relation. The latter case happens when the last constraint has weakly vanishing Poisson bracket with the primary constraints and the Hamiltonian.

We denote the set of constraints $\Phi^{(1)}, \Phi^{(2)}, ...$ as *secondary constraints* . These are really consequences of primary constraints while the primary constraints, by themselves have their origin in the singularity of the Lagrangian or singularity of the Hessian matrix. In a pure Hamiltonian point of view, however, the origin of primary constraints is not of essential importance. In any way given some primary constraints, we should build the total Hamiltonian, (2.5), and check their consistency.

There is another important classification of constraints: If the Poisson bracket of each constraint with all the constraints in the chain vanishes, they are called *first class constraints.* And if the matrix of mutual Poisson brackets of the constraints, C^{MN}, [3]

$$C^{MN} = \{\Phi_a^{(i)}, \Phi_b^{(j)}\}, \tag{2.8}$$

[3] M, N counts both the indices a and i.

has the maximally rank, it is invertible, we deal with *second class constraints*. It is shown that a constraint chain terminating with an identity, is of first class and ending with determining Lagrange multipliers are of second class [9]. To find the dynamics of a system with second class constraints, one may use the Dirac bracket,

$$\{A, B\}_{D.B.} = \{A, B\}_{P.B.} - \{A, \Phi_M\}_{P.B.} (C^{-1})^{MN} \{\Phi_N, B\}_{P.B.}, \tag{2.9}$$

instead of Poisson bracket. The important property of the Dirac bracket is that for an arbitrary A and for all constraints Φ_M,

$$\{\Phi_M, A\}_{D.B.} = 0. \tag{2.10}$$

So, using the Dirac brackets instead of Poisson bracket, the weak equations may be written as strong equalities.

For second class constraints we can always find a *canonical transformation* such that the constraints, Φ_M, lie on the first $2n$ coordinates $(q_1, ..., q_n; p_1, ..., p_n)$ of the phase space and the remaining degrees of freedom, $(Q_1, ..., Q_{N-n}; P_1, ..., P_{N-n})$ are unconstrained. The Dirac bracket in the original phase space is equal to the Poisson bracket in the space $(Q_1, ..., Q_{N-n}; P_1, ..., P_{N-n})$, the *reduced phase space* [1, 10, 11]. Although finding the above canonical transformation is not an easy task, for the case we study in this paper, boundary conditions as constraints, we show that using the suitable mode expansions, is in fact equivalent to going to reduced phase space.

3 Boundary Conditions as Constraints

Boundary conditions are acceleration free equations which in general are not related to a singular Lagrangian. To visualize this point, let us take a simple (1+1) field theory as a toy model

$$S = \frac{1}{2} \int_0^l dx \int_{t_1}^{t_2} dt \ \ (\partial_t \phi)^2 - (\partial_x \phi)^2. \tag{3.1}$$

Variation of the action with respect to ϕ gives

$$\delta S = \int_0^l dx \int_{t_1}^{t_2} dt \mathbf{L}(\phi) \delta\phi + \int_{t_1}^{t_2} dt (\partial_x \phi) \delta\phi|_0^l + \int_0^l dt (\partial_t \phi) \delta\phi|_{t_1}^{t_2}. \tag{3.2}$$

For an arbitrary $\delta\phi$, variation of the action vanishes if the three terms in the above equation vanish independently. The first term in (3.2) leads to equations of motion and the last term to the initial conditions. The second term which is called the surface term, results in the boundary conditions. For this term to vanish, there are two choices $\delta\phi|_{boundary} = 0$, Dirichlet boundary conditions, or $\partial_x \phi|_{boundary} = 0$, Neumann boundary conditions. The boundary conditions unlike the equations of motion, are acceleration-free equations and should be held at all the times. In other words, they can be treated as Lagrangian constraints. To clarify this point we repeat the above argument in the discrete version:

$$S = \frac{1}{2}\int_{t_1}^{t_2} dt \sum_{i=0}^{N} \epsilon(\partial_t \phi_i)^2 - \sum_{i=0}^{N-1} \frac{1}{\epsilon}(\phi_i - \phi_{i+1})^2, \tag{3.3}$$

$$\phi_i(t) = \phi(x,t)|_{x=x_i} \quad ; x_n = n\epsilon, \tag{3.4}$$

and $\epsilon = \frac{l}{N}$ so that $\epsilon \to 0$ ($N \to \infty$) reproduces the continuum theory.

Demanding the variation of (3.4) to vanish, leads to [4]

$$\begin{aligned} \epsilon\partial_t^2 \phi_0 &= \tfrac{1}{\epsilon}(\phi_1 - \phi_0), \\ \epsilon\partial_t^2 \phi_i &= \tfrac{1}{\epsilon}(\phi_{i+1} - 2\phi_i + \phi_{i-1}), \quad i \neq 0, N \\ \epsilon\partial_t^2 \phi_N &= \tfrac{1}{\epsilon}(\phi_N - \phi_{N-1}). \end{aligned} \tag{3.5}$$

So, the boundary conditions are replaced with *equations of motion* at the end points. Taking the continuum limit, assuming that acceleration of the end point are finite, the equations for $0, N$ give

$$\lim \frac{1}{\epsilon}(\phi_1 - \phi_0) = 0 \quad \text{and} \quad \lim \frac{1}{\epsilon}(\phi_N - \phi_{N-1}) = 0. \tag{3.6}$$

Hence in the continuum limit *equations of motion* for the end points give acceleration free equations, the Lagrangian constraints.

A new feature appearing here is that, unlike the usual Lagrangian constraints, boundary conditions are the constraints which are not a consequence of a singular Lagrangian, but a result of taking the continuum limit.

4 The Hamiltonian Setup

In this section, by going to Hamiltonian formulation, we apply the Dirac procedure to a field theory with given boundary conditions. Again, we take our simple toy model and treat the

[4] It is worth noting that we still have the option $\delta\phi_0$ or $\delta\phi_N = 0$ which in the continuum limit translate into the Dirichlet boundary conditions .

boundary conditions as Hamiltonian primary constraints:

$$\Phi^{(0)} = \partial_x \phi|_{x=0}. \tag{4.1}$$

Here we explicitly work out Neumann boundary condition at one end , the Neumann boundary condition at the other end and the Dirichlet cases can be worked out similarly. The total Hamiltonian is built by adding the constraint to the Hamiltonian by arbitrary Lagrange multiplier

$$H_T = H + \lambda \Phi^{(0)}, \tag{4.2}$$

with

$$H = \frac{1}{2}\int_0^l dx \ \ \Pi^2 + (\partial_x \phi)^2 \quad ; \quad \Pi = \partial_t \phi. \tag{4.3}$$

Now we should check the consistency conditions

$$\dot{\Phi}^{(0)} = \{\Phi^{(0)}, H_T\}_{P.B.} = \partial_x \Pi|_0 \equiv \Phi^{(1)}, \tag{4.4}$$

which leads to the secondary constraint, $\Phi^{(1)}$. It should be noted that to obtain (4.4) we have used $\Phi^{(0)} = \int \delta(x) \partial_x \phi dx$, and although the conditions are imposed at the boundaries, the fields can safely be extended to neighbourhood of the boundaries.

We should go further:

$$\dot{\Phi}^{(1)} = \{\Phi^{(1)}, H_T\} = \{\Phi^{(1)}, H\} + \lambda\{\Phi^{(1)}, \Phi^{(0)}\} = 0. \tag{4.5}$$

The second term on the right hand side,

$$\begin{aligned} \lambda\{\Phi^{(1)}, \Phi^{(0)}\} &= \int \delta(x)\delta(x')\{\partial_x \Pi, \partial_{x'}\phi\} dx dx' \\ &= -\int \delta(x)\delta(x')\partial_x \partial_{x'} \delta(x-x') dx dx', \end{aligned} \tag{4.6}$$

is not well-defined, and formally can be written as $\partial_x^2 \delta(x-x')|_{x=x'=0}$. This term compared to the first term is infinitely large. The only way to make the constraint consistent is

$$\lambda = 0, \tag{4.7}$$

and

$$\{\Phi^{(1)}, H\} = 0. \tag{4.8}$$

There is a new option appearing which is not any of the cases *i)* and *ii)* discussed in section 2. The constraint consistency condition, (4.5), reduces to two equations, (4.7) and (4.8), and although the Lagrange multiplier is determined the constraint chain is not cut.

The above discussion can be better understood if the calculation is regularized by considering the discrete case. Solving the the discrete version of equation (4.5), λ is obtained to be of the order of ϵ, going to the continuum limit is vanishes, and the other term, $\{\Phi^{(1)}, H\}$, should vanish separately.

Defining $\{\Phi^{(1)}, H\}$ as $\Phi^{(2)}$, the other secondary constraint, we find

$$\Phi^{(2)} = \partial_x^3 \phi|_0. \tag{4.9}$$

We should go on:

$$\Phi^{(3)} \equiv \dot{\Phi}^{(2)} = \{\Phi^{(2)}, H_T\} = \{\Phi^{(2)}, H\} = \partial_x^3 \Pi|_0. \tag{4.10}$$

This process should be continued and each time we find a new secondary constraint. Finally we are left with an infinite number of constraints:

$$\Phi^{(n)} = \begin{cases} \partial_x^{(n+1)} \phi|_0 & n = 0, 2, 4, ... \\ \\ \partial_x^{(n)} \Pi|_0 & n = 1, 3, 5, ... \end{cases} \tag{4.11}$$

Exhausted the constraint consistency conditions, we should determine of which class these constraints are. Since the Poisson bracket of the constraints,

$$C_{mn} \equiv \{\Phi^{(m)}, \Phi^{(n)}\}, \tag{4.12}$$

is non-zero, we may be dealing with the second class constraints:

$$C_{mn} = \begin{cases} 0 & m, n = 0, 2, 4, ... \\ \\ 0 & m, n = 1, 3, 5, ... \\ \\ \int \delta(x)\delta(x')\partial_x^{m+1}\partial_{x'}^{n}\delta(x-x')dxdx' & m = 0, 2, 4, ..., n = 1, 3, 5, ... \end{cases} \tag{4.13}$$

To find $detC$, the non-zero elements should be regularized. This regularization can be done by two methods, discretization or using a limit of a regular function, e.g. the Gaussian function, instead of $\delta(x)$. Here we choose the second, but one can easily show that the other method gives the same results. Inserting

$$\delta(x-x') = \lim_{\epsilon \to 0} \frac{1}{\epsilon\sqrt{\pi}} e^{\frac{-(x-x')^2}{\epsilon^2}} \tag{4.14}$$

into (4.13) we find

$$\begin{aligned} &\int \delta(x)\delta(x')\partial_x^{m+1}\partial_{x'}^{n}\delta(x-x')dxdx' = \tfrac{-1}{\sqrt{\pi}}\epsilon^{-(m+n+2)} H_{m+n+1}(0) \\ &= \tfrac{-1}{\sqrt{\pi}}(-2)^{(n+m+1)/2}\epsilon^{-(m+n+2)}(m+n)!!, \quad m = 0, 2, 4, ..., n = 1, 3, 5, ... \end{aligned} \tag{4.15}$$

$H_n(0)$ denotes the Hermite polynomials calculated at $x = 0$. Putting all of these together, finally C is found to be

$$C = A \otimes B, \tag{4.16}$$

where

$$A = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},$$

and B is an infinite dimensional matrix with

$$B_{mn} = \frac{-1}{\sqrt{\pi}}(-2)^{(n+m-1)} \frac{((2(m+n)-3)!!}{\epsilon^{-2(m+n)-1}} \qquad m, n = 1, 2, ... \tag{4.17}$$

It is a straight-forward calculation to show that the B matrix has non-zero determinant, i.e. the C matrix is invertible, and hence all the constraints in the chain are second class. One way to consider all of them is using the Dirac bracket. To find Dirac bracket of any two arbitrary functions in the phase space, it is enough to have Dirac brackets of (ϕ, ϕ) , (ϕ, Π) and (Π, Π)

$$\{\phi(x), \phi(x')\}_{D.B.} = -\{\phi(x), \Phi^{(m)}\}C^{-1}_{mn}\{\Phi^{(n)}, \phi(x')\} = 0. \tag{4.18}$$

$$\{\Pi(x), \Pi(x')\}_{D.B.} = -\{\Pi(x), \Phi^{(m)}\}C^{-1}_{mn}\{\Phi^{(n)}, \Pi(x')\} = 0. \tag{4.19}$$

$$\begin{aligned} \{\phi(x), \Pi(x')\}_{D.B.} &= \delta(x - x') - \{\phi(x), \Phi^{(m)}\}C^{-1}_{mn}\{\Phi^{(n)}, \Pi(x')\} \\ &= \delta(x - x') - R(x, x'). \end{aligned} \tag{4.20}$$

Without having the explicit form of C^{-1} we can show that[5]

$$R(x, x') = \kappa\epsilon\delta(x)\delta(x'), \tag{4.21}$$

where κ is a numeric factor. To find κ, let us calculate Dirac bracket of constraints with an arbitrary function f, using (2.10) we have

$$\{\partial_x\phi(x)|_0, f(\phi, \Pi)\}_{D.B.} = \int \delta(x)\partial_x\{\phi(x), f\}_{D.B.} = 0. \tag{4.22}$$

Calling $\frac{\partial f}{\partial \Pi(x')}$, $g(x')$

$$\int \delta(x)\partial_x\{\phi(x), \Pi(x')\}_{D.B.}g(x') = 0. \tag{4.23}$$

Inserting (4.20) and (4.21) into (4.23) reduces to

$$\int (\partial_x\delta(x) + \kappa\epsilon\delta(x)\partial_x\delta(x))g(x) = 0. \tag{4.24}$$

[5]Find more detailed calculations in the appendix.

Remembering (4.14), we find

$$\kappa = -\sqrt{\pi}. \tag{4.25}$$

And hence

$$\{\phi(x), \Pi(x')\}_{D.B.} = \delta(x - x') + \kappa\epsilon\delta(x)\delta(x'). \tag{4.26}$$

Appearance of regularization parameter, ϵ, in the Dirac bracket sounds bad, but since the second term has two delta functions, to be of the same order of the first term, there must be an ϵ factor. We will clarify and discuss this point in the next section.

The Dirichlet boundary condition can be worked out similarly and the only difference is that the κ factor is obtained to be $+\sqrt{\pi}$.

5 Mode expansion and Reduced Phase Space

In previous section we showed that a field theory subjected to Neumann or Dirichlet boundary conditions is a system constrained to an infinite chain of *second class* constraints. For a system with second class constraints, there is a subspace of phase space which is spanned by a set of unconstrained variables, the reduced phase space. The important property of these variables is that, Poisson bracket in terms of them is equal to the Dirac bracket defined on the whole constrained phase space.

In this section we will explicitly find the reduced phase space and show that it is exactly phase space determined by the mode expansion method.

Let us consider the Fourier transformed variables

$$\begin{aligned} \phi(x) &= \tfrac{1}{\sqrt{2\pi}} \int \phi(k) e^{ikx} dk \quad , \quad \phi(k) = \tfrac{1}{\sqrt{2\pi}} \int \phi(x) e^{-ikx} dx \\ \Pi(x) &= \tfrac{1}{\sqrt{2\pi}} \int \Pi(k) e^{-ikx} dk \quad , \quad \Pi(k) = \tfrac{1}{\sqrt{2\pi}} \int \Pi(x) e^{ikx} dx. \end{aligned} \tag{5.1}$$

One can easily show that the above transformation is canonical:

$$\{\phi(k), \phi(k')\} = 0 \ , \quad \{\Pi(k), \Pi(k')\} = 0 \quad , \quad \{\phi(k), \Pi(k')\} = \delta(k - k'). \tag{5.2}$$

The Neumann (Dirichlet), constraints chain in terms of the new variables are easily obtained:

All the odd (even) moments of $\phi(k)$ and $\Pi(k)$ are zero.

The most general solution to the constraints is that $\phi(k)$ and $\Pi(k)$ are even (odd) functions of k. So, imposing the constraints on variable we have [6]

$$\phi(x) = \frac{1}{\sqrt{\pi}} \int \phi(k) \cos kx dk \quad , \qquad \Pi(x) = \frac{1}{\sqrt{\pi}} \int \Pi(k) \cos kx dk. \tag{5.3}$$

$\phi(x)$ and $\Pi(x)$ defined in (5.3) are the variables spanning the reduced phase space.

To compare the Dirac bracket results with those of reduced phase space, we work out Poisson brackets of $\phi(x)$ and $\Pi(x)$, given by (5.3). Assuming (5.2), we have

$$\begin{aligned} \{\phi(x), \phi(x')\} &= \tfrac{1}{\sqrt{\pi}} \textstyle\int \{\phi(k), \phi(k')\} \cos kx \cos k'x' dk dk' = 0, \\ \{\Pi(x), \Pi(x')\} = \{\Pi(k), \Pi(k')\} &= \tfrac{1}{\sqrt{\pi}} \textstyle\int \{\Pi(k), \Pi(k')\} \cos kx \cos k'x' dk dk' = 0, \\ \{\phi(x), \Pi(x')\} &= \tfrac{1}{\sqrt{\pi}} \textstyle\int \{\phi(k), \Pi(k')\} \cos kx \cos k'x' dk dk' \equiv \delta_N(x, x'), \end{aligned} \tag{5.4}$$

for Neumann boundary conditions and for Dirichlet case only $\{\phi, \Pi\}$ differs from above:

$$\{\phi(x), \Pi(x')\} = \frac{1}{\sqrt{\pi}} \int \sin kx \sin k'x' dk dk' \equiv \delta_D(x, x'). \tag{5.5}$$

Performing the integrations we have

$$\begin{aligned} \delta_N(x, x') &= \delta(x - x') + \delta(x + x'), \\ \delta_D(x, x') &= \delta(x - x') - \delta(x + x'). \end{aligned} \tag{5.6}$$

If we consider only the positive x's, $x \geq 0$, δ_N and δ_D for $x, x' \neq 0$ is exactly $\delta(x - x')$. For $x, x' = 0$, we regularize delta functions by

$$\begin{cases} \delta(x - x') + \delta(x + x') = \frac{2}{\sqrt{\pi}\epsilon}, \\ \delta(x - x') - \delta(x + x') = 0. \end{cases} \qquad \text{at } \; x = x' = 0 \tag{5.7}$$

Hence δ_N and δ_D for $x \geq 0$ is in exact agreement with the Dirac bracket results obtained in previous section. The above argument clarifies, why using the usual mode expansions to quantize a system with Neumann or Dirichlet boundary condition, i.e. , imposing the boundary conditions and *then* quantizing, works.

[6] For Dirichlet case Cosine should be replaced be Sine.

6 Mixed Boundary Conditions, Another Example

In this section we handle a more general family of boundary conditions, mixed boundary conditions, which are a combination of Neumann and Dirichlet cases. It has been shown that these boundary conditions lead to unusual results in the context of string theory [2, 3, 4, 5, 6, 7].

As a toy model for a field theory resulting in the mixed boundary conditions consider

$$S = \frac{1}{2}\int_0^l dx \int_{t_1}^{t_2} dt[(\partial_t\phi_i)^2 - (\partial_x\phi_i)^2 + F_{ij}\partial_t\phi_i\partial_x\phi_j], \tag{6.1}$$

where $i, j = 1, 2$ and F_{ij} is a constant antisymmetric background. Variation of S with respect to ϕ_i, gives:

$$\partial_t^2\phi_i = \partial_x^2\phi^i, \tag{6.2}$$

$$\partial_x\phi_i + \mathcal{F}_{ij}\partial_t\phi_j = 0 \quad \text{at} \;\; x = 0, l. \tag{6.3}$$

Equations (6.3), as discussed in section 3, give the Lagrangian constraints. In the discretized version, (6.3) are the equations of motion for the end points and in the continuum limit, the acceleration term disappears. It is worth noting that (6.3) reproduce the Neumann and Dirichlet boundary conditions for $F = 0$ and ∞ respectively.

Now to apply the Dirac method, we go to Hamiltonian formulation:

$$\Pi_i = \partial_t\phi_i + \mathcal{F}_{ij}\partial_x\phi_j, \tag{6.4}$$

$$H = \frac{1}{2}\int_0^l (\Pi_i - F_{ij}\partial_x\phi_j)^2 + (\partial_x\phi_i)^2 \;\; dx, \tag{6.5}$$

and the primary constraints,

$$\Phi_i^{(0)} = \Phi_i(x)|_{x=0}, \tag{6.6}$$

with

$$\Phi_i(x) \equiv M_{ij}\partial_x\phi_j + \mathcal{F}_{ij}\Pi_j = 0 \;\; , \;\; M_{ij} = (\mathbf{1} - F^2)_{ij}. \tag{6.7}$$

To obtain (6.6), note that since the constraints are not a consequence of singular Lagrangian (sec. 3), we are allowed to rewrite constraints in terms of canonical variables, using (6.4).

The consistency of the primary constraints should be verified:

$$\dot{\Phi}_i^{(0)} = \{\Phi_i^{(0)}, H_T\} = \{\Phi_i^{(0)}, H\} + \lambda_j\{\Phi_i^{(0)}, \Phi_j^{(0)}\} = 0. \tag{6.8}$$

The first term is easy to work out:

$$\Phi_i^{(1)} = \{\Phi_i^{(0)}, H\} = \partial_x\Pi_i|_{x=0}. \tag{6.9}$$

As argued in sec. 4, $\{\Phi_i^{(0)}, \Phi_j^{(0)}\}$ is infinitely large compared to the first term, and the only way for (6.8) to be satisfied is

$$\lambda_i = 0 \quad \text{and} \quad \Phi_i^{(1)} = 0. \tag{6.10}$$

Similar to previous cases, although the Lagrange multiplier, λ_i, is determined, there are secondary constraints, $\Phi_i^{(1)} = 0$. Moreover we have the advantage that λ_i disappears in the remaining steps.

The consistency conditions for the constraints leads to the chain

$$\Phi_i^{(n)} = \begin{cases} \partial_x^n \Phi_i|_0 & n = 0, 2, 4, ... \\ \\ \partial_x^{(n)} \Pi_i|_0 & n = 1, 3, 5, ... \end{cases} \tag{6.11}$$

To verify that these constraints are really second class, we study the C matrix, $C_{ij}^{mn} \equiv \{\Phi_i^{(m)}, \Phi_j^{(n)}\}$.

$$C_{ij}^{mn} = \begin{cases} 0 & m, n = 1, 3, 5, ... \\ \\ -2(MF)_{ij} \int \delta(x)\delta(x')\partial_x^{m+1}\partial_{x'}^n \delta(x - x')dxdx' & m, n = 0, 2, 4, ... \\ \\ M_{ij} \int \delta(x)\delta(x')\partial_x^{m+1}\partial_{x'}^n \delta(x - x')dxdx' & m = 0, 2, 4, ..., n = 1, 3, 5, ... \end{cases} \tag{6.12}$$

C can be written in the form of

$$C = F \otimes B, \tag{6.13}$$

where F is a 4×4 matrix:

$$F = \begin{pmatrix} -2(MF)_{ij} & M_{ij} \\ \\ -M_{ij} & 0 \end{pmatrix}, \tag{6.14}$$

and B given by (4.17). In section 4, we discussed that B is invertible and since $det\ F \neq 0$, C is invertible too, and hence all the constraints in the chain (6.11) are second class.

Now let us work out the basic Dirac brackets

$$\begin{aligned} \{\phi_i(x), \phi_j(x')\}_{D.B.} &= -\{\phi_i(x), \Phi_k^{(m)}\}(C^{-1})_{kl}^{mn}\{\Phi_l^{(n)}, \phi_j(x')\} \\ &= (-2M^{-1}F)_{ij}(\epsilon^2\sqrt{\pi}\delta(x)\delta(x')) \end{aligned} \tag{6.15}$$

$$\{\Pi_i(x), \Pi_j(x')\}_{D.B.} = -\{\Pi_i(x), \Phi_k^{(m)}\}(C^{-1})_{kl}^{mn}\{\Phi_l^{(n)}, \Pi_j(x')\} = 0. \tag{6.16}$$

$$\{\phi_i(x), \Pi_j(x')\}_{D.B.} = \delta(x-x') - \{\phi_i(x), \Phi_k^{(m)}\}(C^{-1})_{kl}^{mn}\{\Phi_l^{(n)}, \Pi_j(x')\}$$
$$= \delta(x-x') - R(x,x') = \delta_N(x,x'). \tag{6.17}$$

The important result of the mixed case is (6.15); the Dirac bracket of two field components are non-zero. This means that in the quantized theory these field components are noncommuting. In the string theory, where the fields describe the space coordinates, (6.15) tells us that, the space probed by open strings with mixed boundary conditions is a *non-commutative* space [2, 3, 4].

Using the canonical (or Fourier) transformations, (5.1) and (5.2), we can explicitly build the reduced phase space for the mixed case.

Defining $\Phi_i(k)$ as the Fourier modes of $\Phi_i(x)$, (6.7),

$$\Phi(x) = \frac{1}{\sqrt{2\pi}}\int \Phi(k)e^{ikx}dk \quad , \quad \Phi(k) = \frac{1}{\sqrt{2\pi}}\int \Phi(x)e^{-ikx}dx, \tag{6.18}$$

using (5.2), Poisson brackets of $\Phi_i(k)$ and $\Pi_i(k)$ can be worked out.

Imposing the constraints (6.11), we find that $\Phi_i(k)$ and $\Pi_j(k)$, are odd and even functions of k respectively:

$$\Phi_i(x) = \frac{1}{\sqrt{\pi}}\int \Phi_i(k)\sin kxdk \quad , \quad \Pi(x) = \frac{1}{\sqrt{\pi}}\int \Pi(k)\cos kxdk. \tag{6.19}$$

Remembering (6.7), we can calculate the field components:

$$\phi_i(x) = \frac{M_{ij}^{-1}}{\sqrt{\pi}}\int \frac{-dk}{k}(\Phi_j(k)\cos kx + F_{jk}\Pi_k(k)\sin kx), \tag{6.20}$$

which explicitly satisfies the mixed boundary conditions.

Having found the mode expansions of the fields and their conjugate momenta, we build the Poisson brackets of them

$$\{\phi_i(x), \phi_j(x')\} = \tfrac{1}{\pi}\int \tfrac{dk}{k}\tfrac{dk'}{k'}[(M^{-1}F)_{ik}\{\Phi_k(k), \Pi_l(k')\}M_{lj}^{-1}\cos kx\sin k'x' +$$
$$+(M^{-1}F)_{jk}\{\Pi_k(k), \Phi_l(k')\}M_{il}^{-1}\cos k'x'\sin kx]$$
$$= \tfrac{-1}{\pi}\int \tfrac{dk}{k}(M^{-1}F)_{ij}(\cos kx'\sin kx + \cos kx\sin kx') \tag{6.21}$$
$$= (M^{-1}F)_{ij}\int^x(\delta_N(x,x') - \delta_D(x,x'))dx$$
$$= -2(M^{-1}F)_{ij}\int^x \delta(x+x')dx.$$

Since for $x, x' \geq 0$

$$\int^{x} \delta(x + x')dx = \begin{cases} 1 & x = x' = 0 \\ \\ 0 & otherwise, \end{cases} \tag{6.22}$$

(6.21) is non-zero only for $x, x' = 0$:

$$\{\phi_i(0), \phi_j(0)\} = -2(M^{-1}F)_{ij}. \tag{6.23}$$

Comparing (6.21) and (6.15), we find that they are exactly the same. In other words, (6.19) and (6.20) are functions defining the reduced phase space.

We can also calculate $\{\Pi_i(x), \Pi_j(x')\}$ and $\{\phi_i(x), \Pi_j(x')\}$, and they are obtained to be in exact agreement with (6.16) and (6.17).

7 Concluding Remarks

In this article, we studied the old and well-known question of field theories with boundary conditions. We discussed that in the Lagrangian formulation boundary conditions are Lagrangian constraints which are not a consequence of a singular Lagrangian. For further study we built the Hamiltonian formulation, and considered boundary conditions as primary constraints. Asking for the constraints consistency conditions we found two new features in the context of constrained systems

1) Although the Lagrange multiplier in the total Hamiltonian is determined, the constraints chain is continued.

2) Boundary conditions are equivalent to an *infinite* chain of *second class* constraints.

Building the Dirac brackets of the fields and their conjugate momenta for these second class constraints, we showed that the method based on mode expansion and equations of motion, is equivalent to working in the reduced phase space.

The relation between Hamiltonian method we built here and the usual method of imposing boundary conditions in the equations of motion, can simply be understood. In the first to ensure that boundary conditions are zero, we make the Taylor expansion of boundary conditions as a function of time, and put all the coefficient equal to zero. These coefficients are exactly our constraints chain. But, in the second, the Fourier mode expansion is used and boundary conditions are guaranteed by choosing all the Fourier components to satisfy boundary conditions.

In the last section of the paper, we handled the mixed boundary conditions which seems to be an exciting problem in the context of string theory [7]. Having noncommuting field components, is the interesting feature appearing in this case. Besides the string theory, mixed boundary conditions can happen in the context of electrodynamics having an extra θ-term:

$$S = \frac{1}{4}\int (\mathcal{F}_{\mu\nu}^2 + \theta\epsilon_{\mu\nu\alpha\beta}\mathcal{F}_{\mu\nu}\mathcal{F}_{\alpha\beta}).$$

In the above action θ plays the role of F in our toy model. Variation of the action leads to a surface term, vanishing of which gives the mixed boundary conditions. Quantizing this theory is an interesting problem we postpone it to future works.

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Appendix: Some of the calculation details

$$K^{(m)}(x) \equiv \{\phi(x), \Phi^{(m)}\} = \begin{cases} 0 & m = 0, 2, 4, ... \\ \{\phi(x), \partial_x^m \Pi^{(m)|_0}\} = k^m(x) & m = 1, 3, 5, ... \end{cases}$$

$$L^{(m)}(x) \equiv \{\Pi(x), \Phi^{(m)}\} = \begin{cases} \{\Pi(x), \partial_x^m \phi^{(m)|_0}\} = l^m(x) & m = 0, 2, 4, ... \\ 0 & m = 1, 3, 5, ... \end{cases}$$

$$k^m(x) = \int \partial_{x'}^m \delta(x - x')\delta(x')dx' = \frac{1}{\sqrt{\epsilon\pi}} exp(\frac{-x^2}{\epsilon^2})\ \frac{1}{\epsilon^m} H_m(0) \equiv \delta(x)k_m.$$

$$l^m(x) = -\int \partial_{x'}^{m+1} \delta(x' - x)\delta(x')dx' = \frac{1}{\sqrt{\epsilon\pi}} exp(\frac{-x^2}{\epsilon^2})\ \frac{1}{\epsilon^{m+1}} H_{m+1}(0) \equiv \delta(x)k_{m+1}.$$

In the above relations, $H_m(0)$ are the Hermite polynomials at zero. Now we can easily work out $\{\phi(x), \Pi(x')\}_{D.B.}$

$$\{\phi(x), \Pi(x')\}_{D.B.} = \delta(x - x') + k_{m+1}k_n B^{-1}_{mn}\delta(x)\delta(x')$$

The power of ϵ in $k_{m+1}k_n B^{-1}_{mn}$, can be read from the explicit form of k_m and B_{mn}, and the results is $k_{m+1}k_n B^{-1}_{mn} = \kappa\epsilon$.

Calculations for the mixed boundary conditions can be performed similarly.

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